Some idea on quantum tunneling from Lefschetz thimbles

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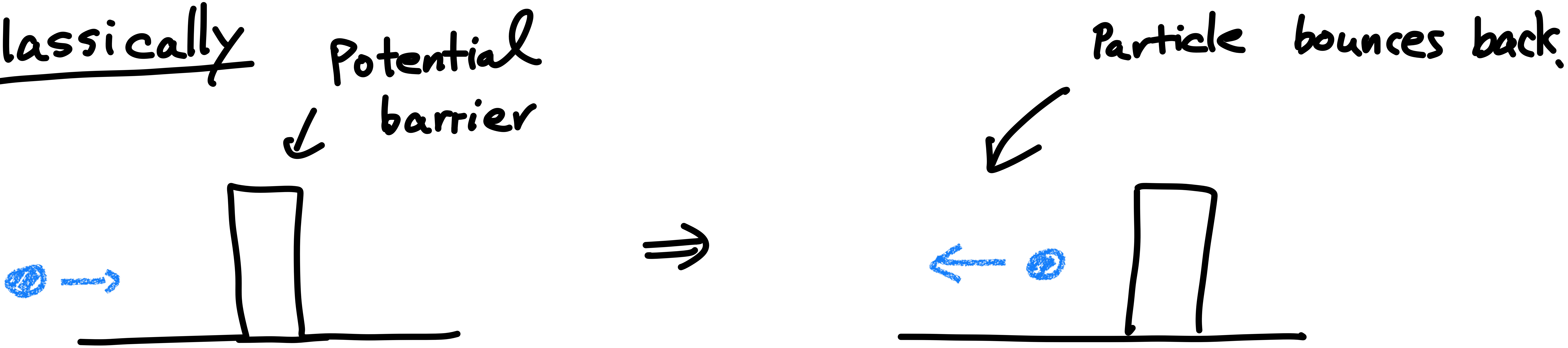
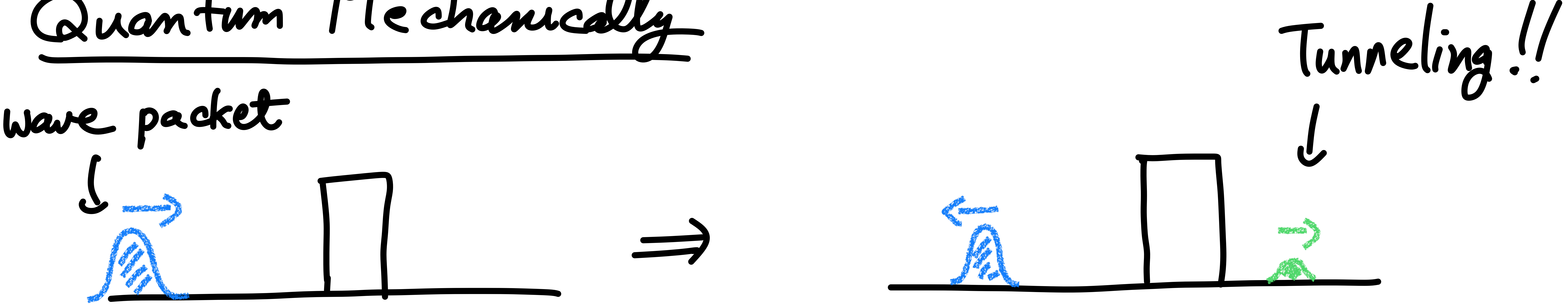
Based on 1406.2386 with Takayuki Koike

Quantum Tunneling

Classically



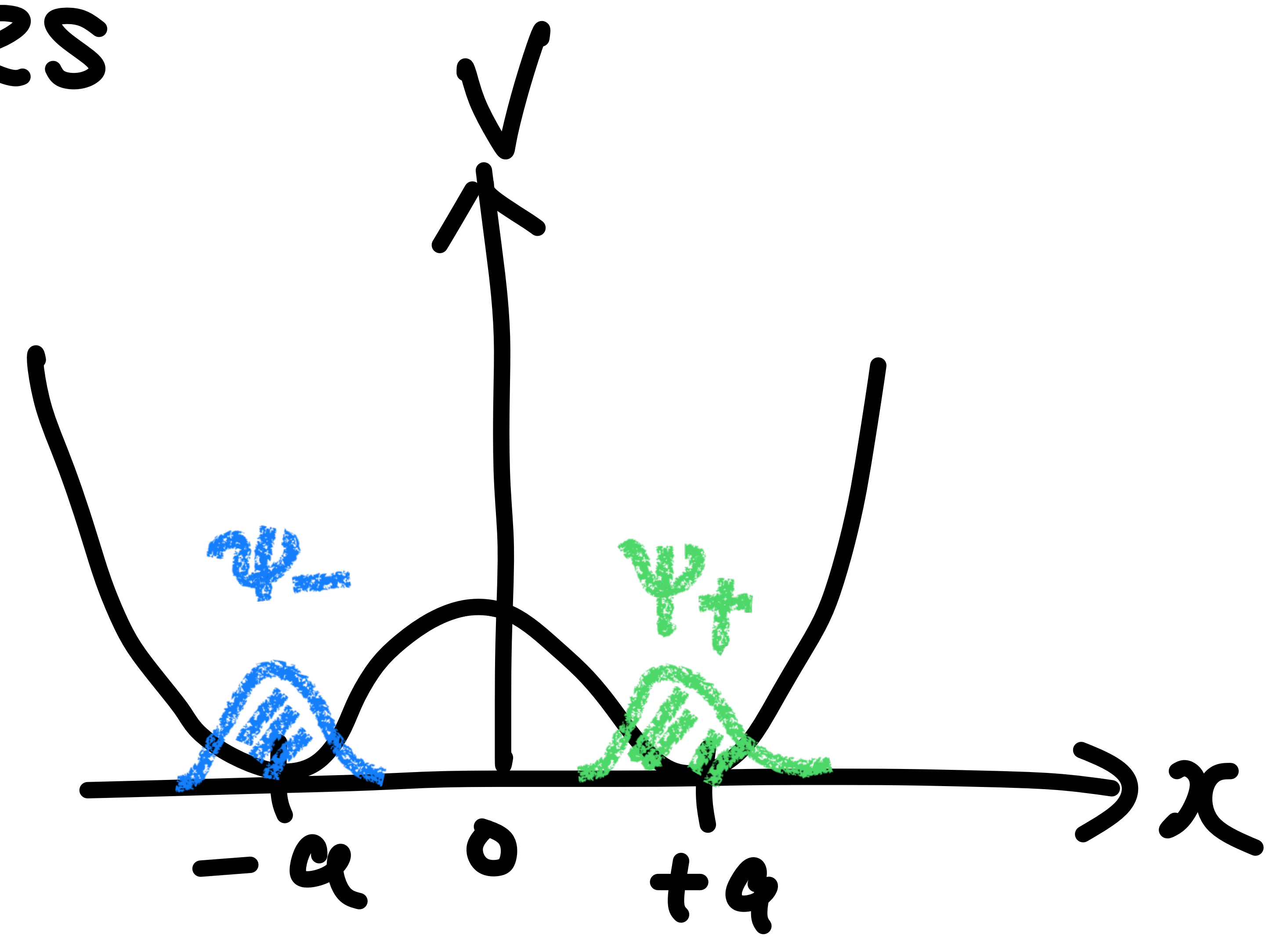
Quantum Mechanically



Tunneling and Ground States

Let's consider G.S. for the double well

$$\hat{H} = -\frac{1}{2}\partial_x^2 + \underbrace{\frac{g}{4}(x^2-a^2)^2}_{V(x)} .$$



Classical vacua of $V(x)$: $x = \pm a$ $\quad (V(\pm a) = 0)$.

So, are there <u>two</u> ground states, ψ_+ and ψ_- ?

<u>No</u> $\psi_{G.S.} \simeq \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$ is the true one!

Why is this so?

<u>Standard trick</u>

- Consider the (imaginary-time) operator: $e^{-\beta \hat{H}}$.

  G.S. of $\hat{H}$ $\Leftrightarrow$ Maximal eigenstate of $e^{-\beta \hat{H}}$.

- Assume $|\Psi_\pm\rangle$ are good approximation of low-E spectra.

  Then, compute 2×2 transition matrix:

$$\begin{pmatrix} \langle \Psi_+ | e^{-\beta \hat{H}} | \Psi_+ \rangle & \langle \Psi_+ | e^{-\beta \hat{H}} | \Psi_- \rangle \\ \langle \Psi_- | e^{-\beta \hat{H}} | \Psi_+ \rangle & \langle \Psi_- | e^{-\beta \hat{H}} | \Psi_- \rangle \end{pmatrix} \simeq \begin{pmatrix} 1 & c \\ c & 1 \end{pmatrix}$$

(annotation: $c \to 0$)

- Now, let's diagonalize the 2x2 matrix $\begin{pmatrix} 1 & c \\ c & 1 \end{pmatrix}$:

$$|\psi_{G.S}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \text{eigenvalue} = 1+C \simeq e^{-\beta E_{G.S.}}$$

(upper entry $\leftarrow |\psi_+\rangle$, lower entry $\leftarrow |\psi_-\rangle$)

$$|\psi_{1st}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \text{eigenvalue} = 1-c \simeq e^{-\beta E_{1st.}}$$

- $\Delta E = E_{1st} - E_{G.S.} \ll 1$.

$$\rightsquigarrow \Delta E = \frac{1}{2\beta} C = \frac{1}{2\beta} \langle \psi_+ | e^{-\beta \hat{H}} | \psi_- \rangle \sim \frac{1}{2} e^{-\frac{S_{inst}}{\hbar}} .$$

($\langle \psi_+ | e^{-\beta \hat{H}} | \psi_- \rangle$: instanton amplitude $\sim \beta e^{-S_{inst}/\hbar}$)

Tunneling and imaginary time (Instanton)

Real-time propagation

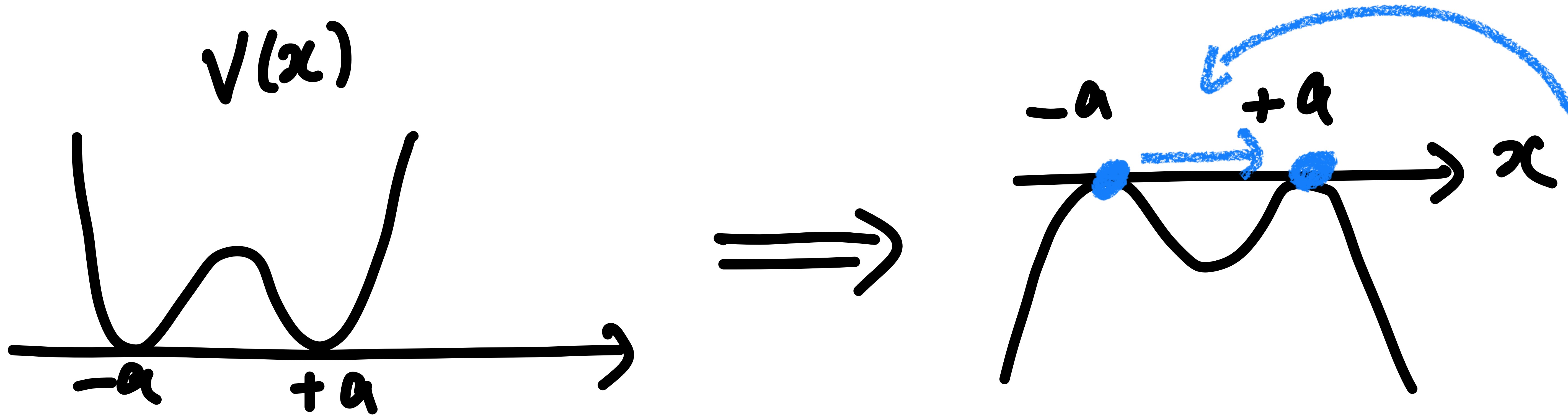
$$\langle \psi_+ | e^{-i\hat{H}T} | \psi_- \rangle = \int \mathcal{D}x \; \exp\left(i \int_0^T dt \left\{ \frac{1}{2} \left(\frac{\partial x}{\partial t} \right)^2 - V(x) \right\} \right).$$

Imaginary time

$$\Downarrow \quad t \to -i\tau \, , \quad T \to -i\beta$$

$$\langle \psi_+ | e^{-\hat{H}\beta} | \psi_- \rangle = \int \mathcal{D}x \, \exp\left(- \int_0^\beta d\tau \left\{ \frac{1}{2} \left(\frac{\partial x}{\partial \tau} \right)^2 + V(x) \right\} \right).$$

Potential is inverted.



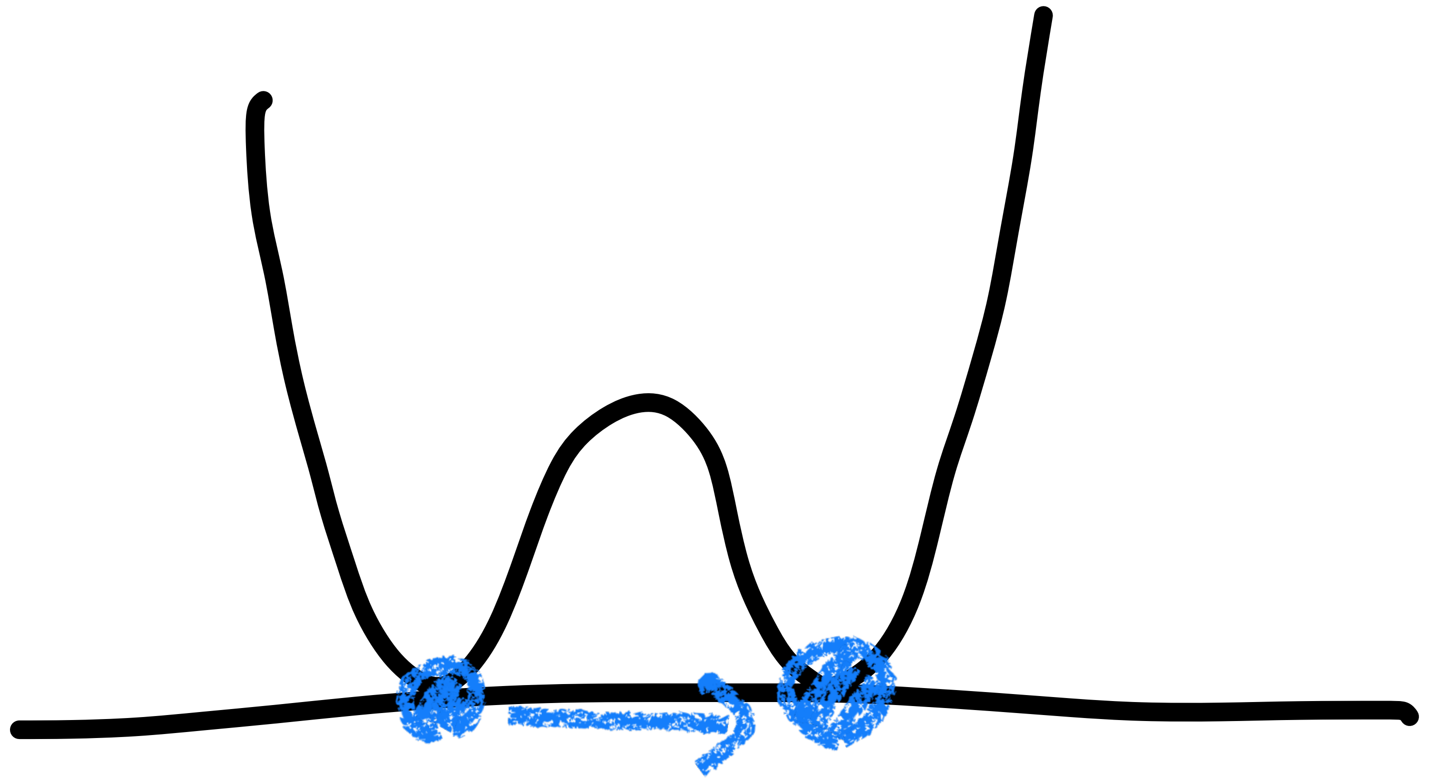
This classical solution is the instanton.

Everything looks nice.

What's the problem?

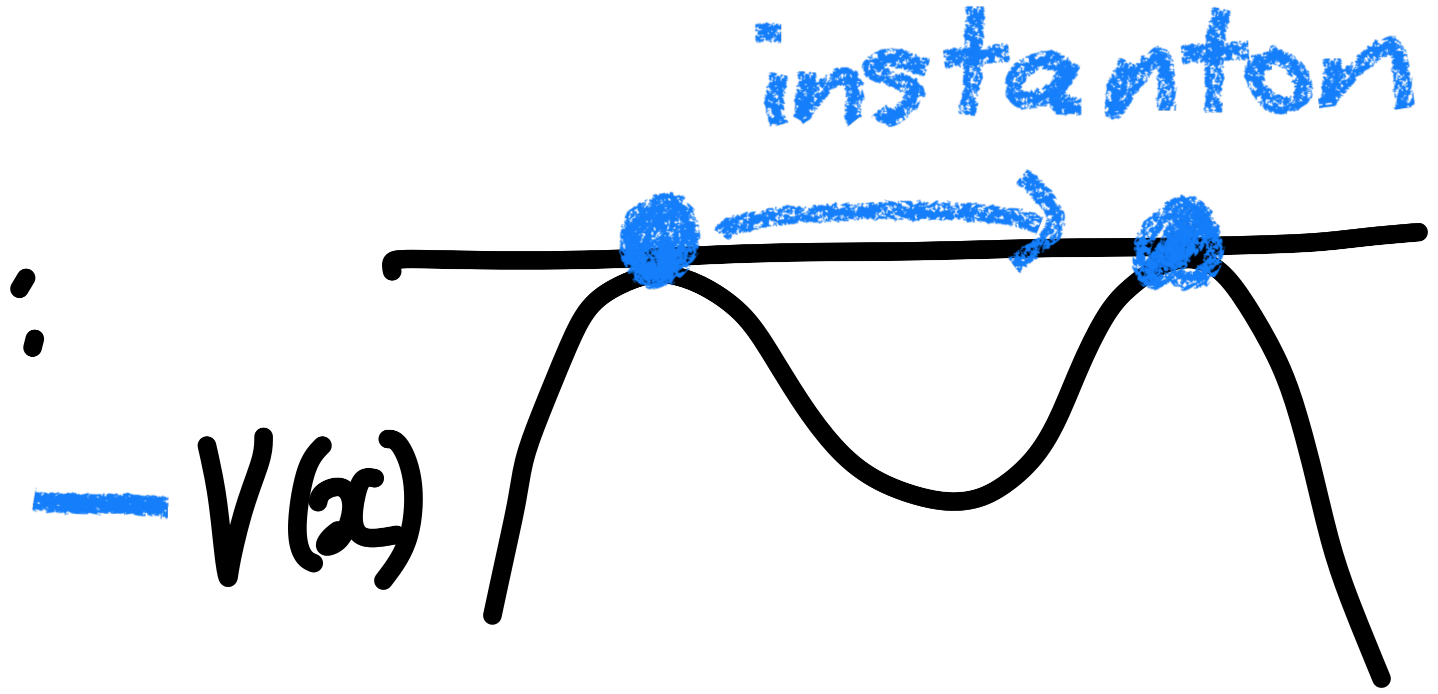
Q.) Can we understand the tunneling in real-time path integral?

⤳ This is quite difficult.



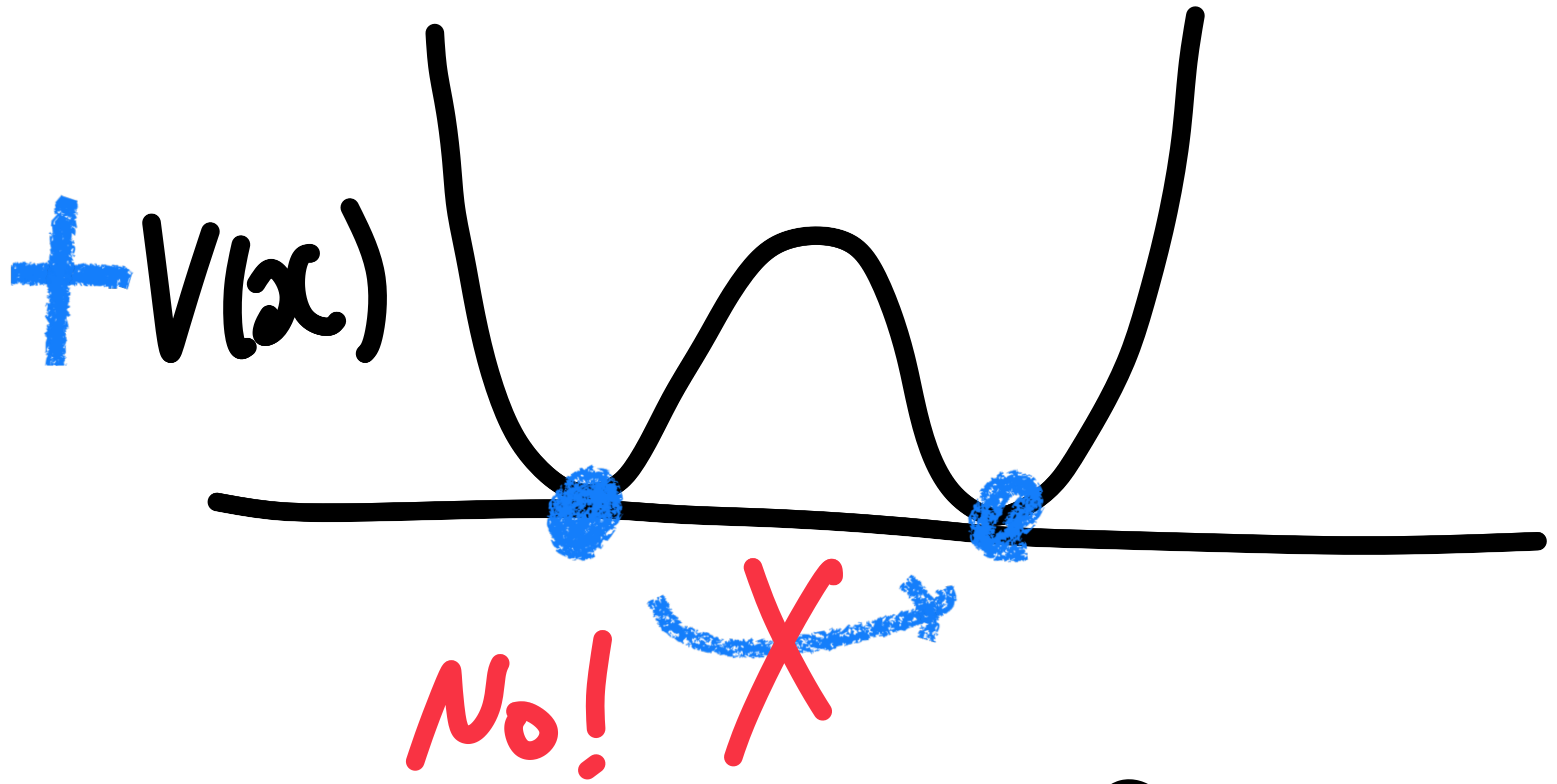
Such a Real classical solution does not exist.

Imaginary-time :



⇝ Quantum tunneling is a semiclassical phenomenon.

Real-time :



⇝ No semiclassical way for tunneling.

Isn't this puzzling?

Lefschetz-thimble path integral

Oscillatory integrals $\Rightarrow \sum_\sigma$ (non-oscillatory integrals)

Around 2013-, Lefschetz-thimble method starts getting attention for the sign problem. (Christoforetti, et al '13; Fujii, et al '13-, ... (Witten '10))

$$\int_{\mathbb{R}^{[0,T]}} \mathcal{D}x\, e^{iS[x]} = \sum_{\sigma:\text{ complex classical sol.}} n_\sigma \int_{J_\sigma} \mathcal{D}z\, e^{iS[z]}.$$

↖ Lefschetz thimble ≈ stationary path.

Assume we are interested in the integral

$$Z = \int_{\mathcal{M}} d^n x \ \exp\left(\frac{1}{\hbar} I(x)\right)$$

($\mathcal{M} = \mathbb{R}^{[0,T]}$, $I(x) = i\,S[x]$ in the real-time path integral)

Complexification $\mathcal{M} \to \mathcal{M}_{\mathbb{C}} = \mathcal{M} \otimes \mathbb{C}$, $x \to z = x + iy$

Convergent Region $C_{-T} = \{ z \in \mathcal{M}_{\mathbb{C}} \mid \mathrm{Re}(I(z)) < -T \}$

classical sol. $\frac{\partial I}{\partial z} = 0$

Then, Lefschetz thimbles $J_\sigma = \left\{ z(0) \in \mathcal{M}_{\mathbb{C}} \;\middle|\; \frac{dz}{dt} = -\overline{\left(\frac{\partial I}{\partial z}\right)},\ z(-\infty) = z_\sigma \right\}$

form the basis of $H_n(\mathcal{M}_{\mathbb{C}}, C_{-T})$ for $T \gg 1$.

$$\rightsquigarrow Z = \sum_\sigma n_\sigma \int_{J_\sigma} d^n z \ \exp\left(\frac{1}{\hbar} I(z)\right).$$

- Integration on each Lefschetz thimbe behaves as

$$Z_\sigma := \int_{J_\sigma} d^n z \, e^{\frac{1}{\hbar} I(z)} = e^{\frac{1}{\hbar} I(z_\sigma)} A_0 \hbar^{\bullet} \left(1 + a_1 \hbar + \cdots \right)$$

$\rightsquigarrow$ Asymptotic expansion in $\hbar \ll 1$.

Let's apply this method to quantum tunneling!

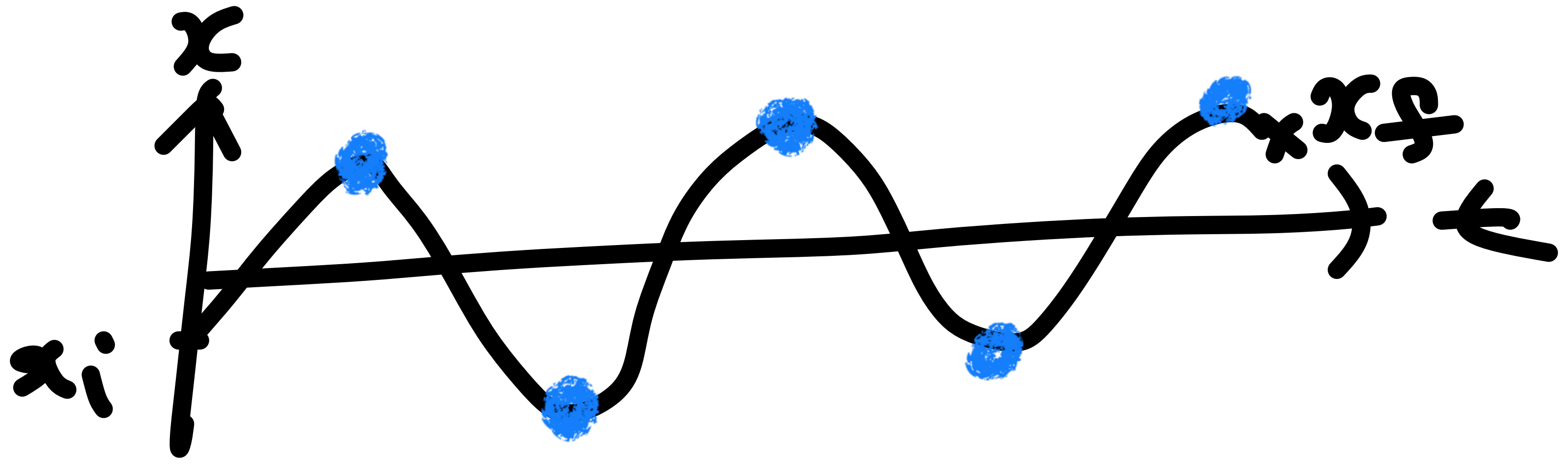
(as it was a semiclassical phenomenon in imaginary time)

(* Use of complex solutions is not a new idea.
But, Lefschetz thimbles may provide a systematic treatment.)

Simple example : Harmonic oscillator

$$I[z] = i\,S[z] = i\int_0^T dt \left\{ \frac{1}{2}\left(\frac{dz}{dt}\right)^2 - \frac{1}{2} z^2 \right\}.$$

$z_{cl} = x_{cl}$



$$\langle x_f | e^{-i\hat{H}T/\hbar} | x_i \rangle = \sqrt{\frac{1}{2\pi i \hbar\, |\sin(T)|}}\; e^{\frac{I(z_{cl})}{\hbar}} \times e^{-i\frac{\pi}{2}\nu}$$

← Maslov index $= \lfloor \frac{T}{\pi} \rfloor$

$\int \mathcal{D}x \Rightarrow \int_J \mathcal{D}z$ produces the correct phase factor.

Path toward quantum tunneling

Double-well : $I[z] = i\,S[z] = i\int dt \left(\frac{1}{2}\left(\frac{dz}{dt}\right)^2 - \frac{1}{2}(z^2-1)^2\right).$

Let's look at behaviors of complex classical solutions.

Energy conservation :

$$\left(\frac{dz}{dt}\right)^2 + (z^2-1)^2 = p^2$$

(complex) energy → p^2

$$\Longrightarrow \quad z(t) = \sqrt{\frac{p^2-1}{2p}}\ \mathrm{sd}\left(\sqrt{2p}\,t + c,\ \sqrt{\frac{1+p}{2p}}\right)$$

sd ↑ Jacobi elliptic func.

k : elliptic modulus $= \sqrt{\frac{1+p}{2p}}$

Elliptic function enjoys double periodicity

$\rightsquigarrow$ Set of "classical" paths $x_i \to x_f$ in time T

$$= \Big\{ (n,m) \in \mathbb{Z}^2 \quad \text{s.t.} \quad n\,\omega_1(k) + m\,\omega_3(k) = \frac{T}{2} + (\text{func. of } x_i, x_f, k) \Big\}.$$

with

$$\omega_1(k) = \sqrt{\frac{2k^2-1}{2}}\, K(k), \quad \omega_3(k) = i\sqrt{\frac{2k^2-1}{2}}\, K\left(\sqrt{1-k^2}\right).$$

← complete elliptic integral.

Which solution is responsible for tunneling?

My first naive guess :

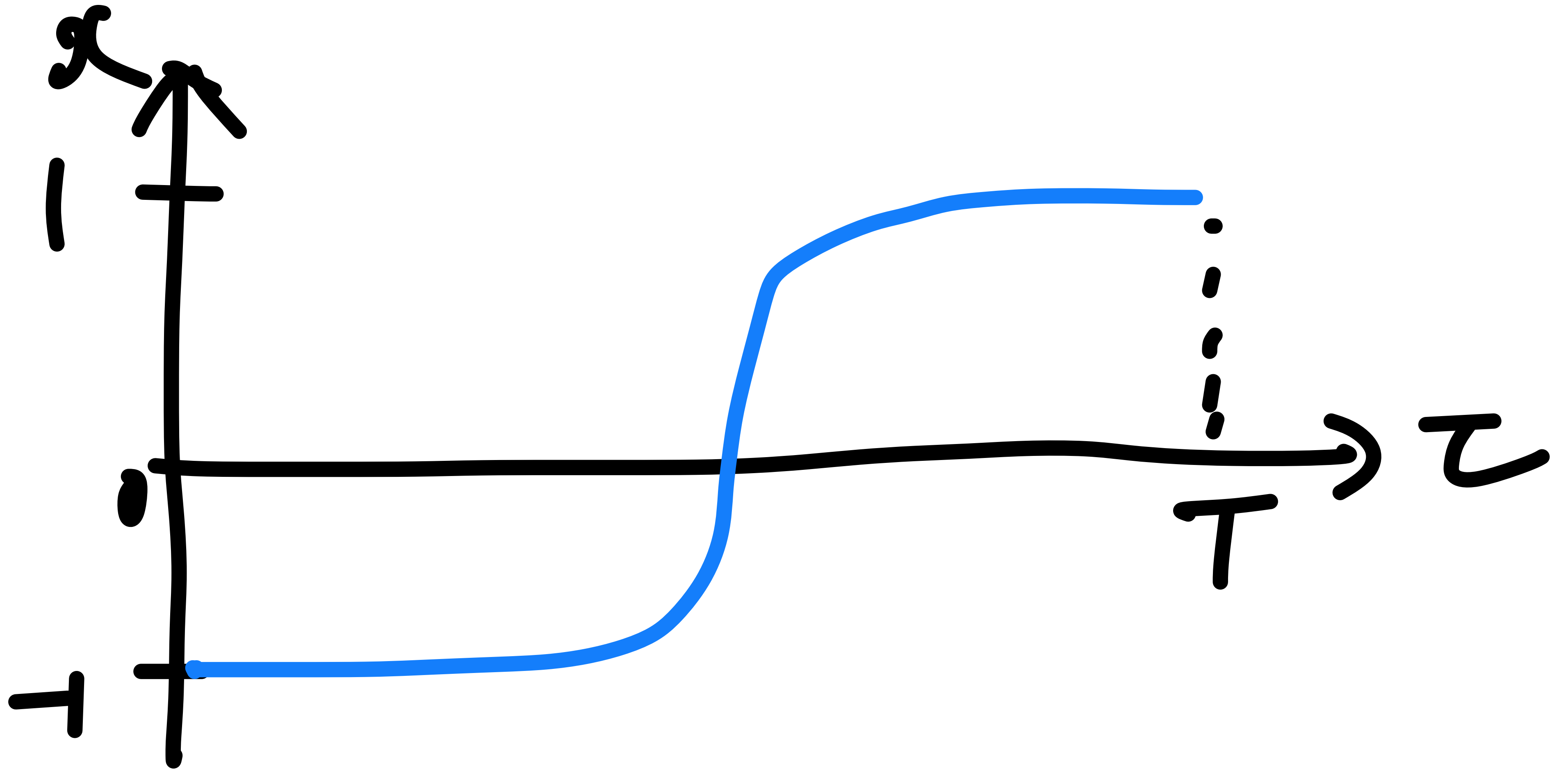
Imaginary-time instanton ⟶ real-time tunneling ?

No!

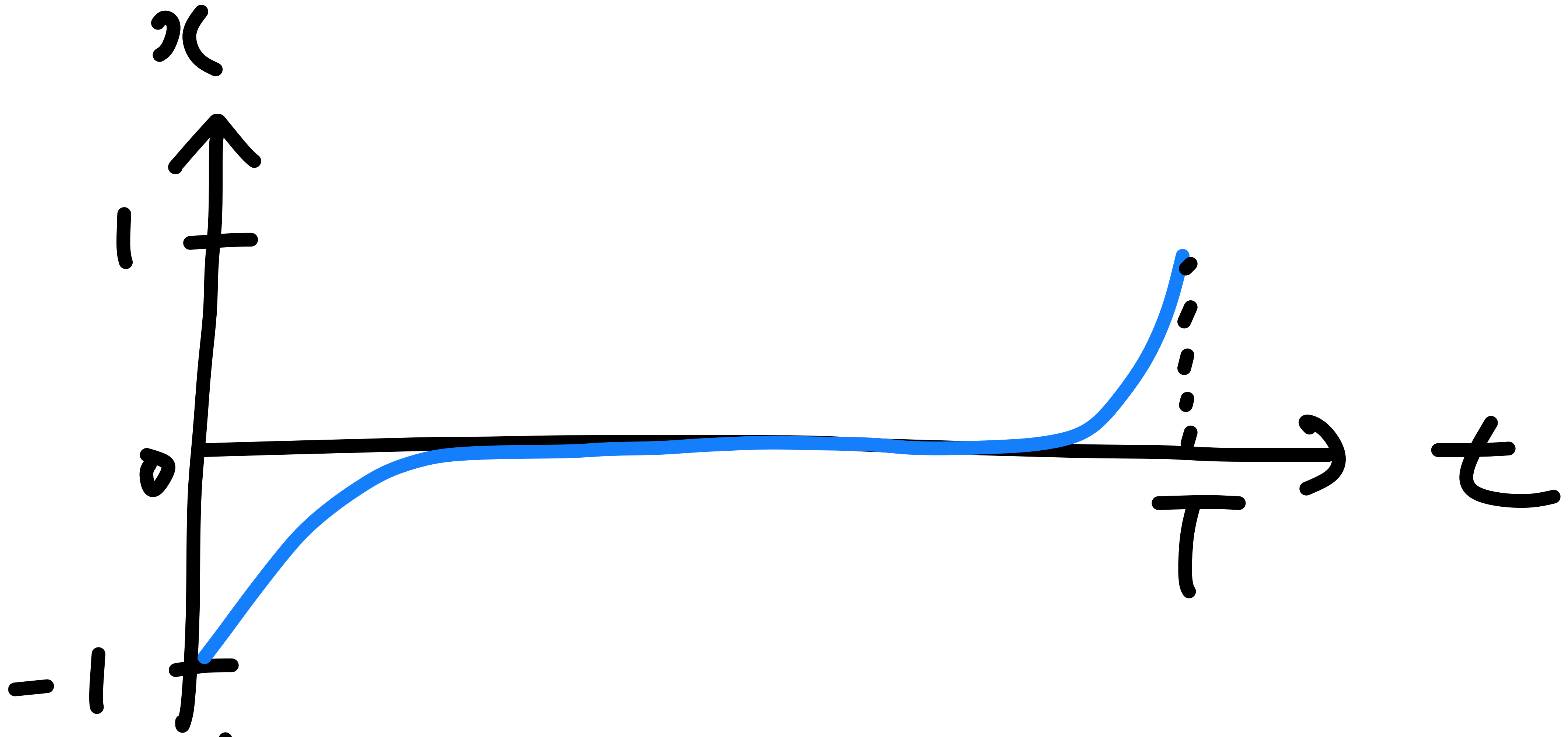
n=m=0

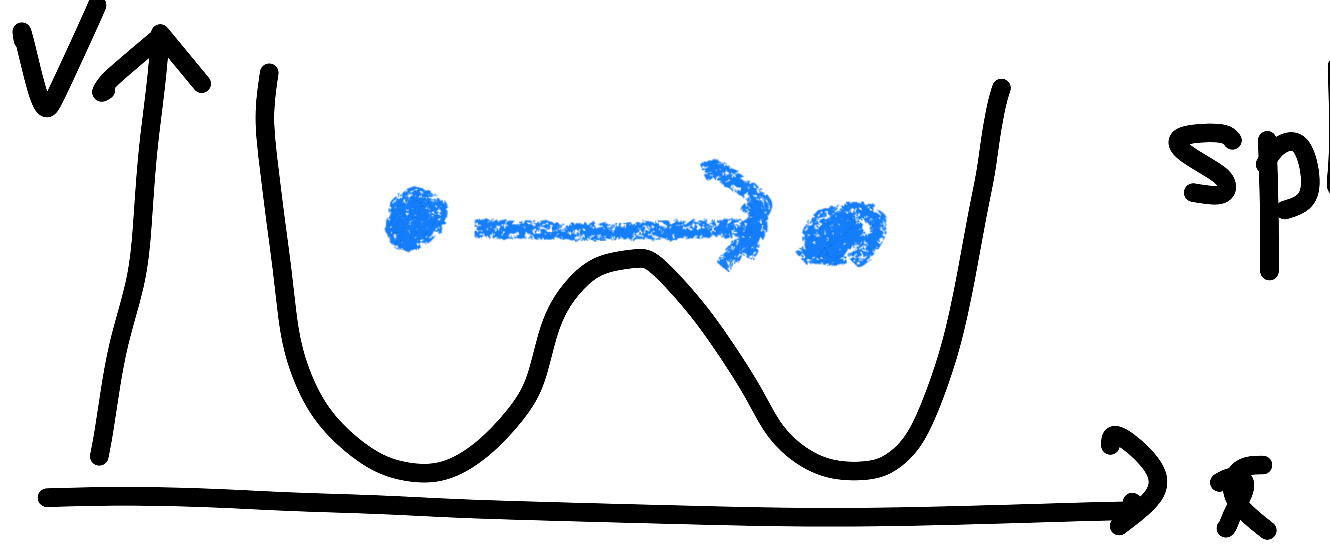
$E = \frac{p^2(t)}{2} \simeq 0$

$E = \frac{p^2(t)}{2} \simeq \frac{1}{2}$



⟶



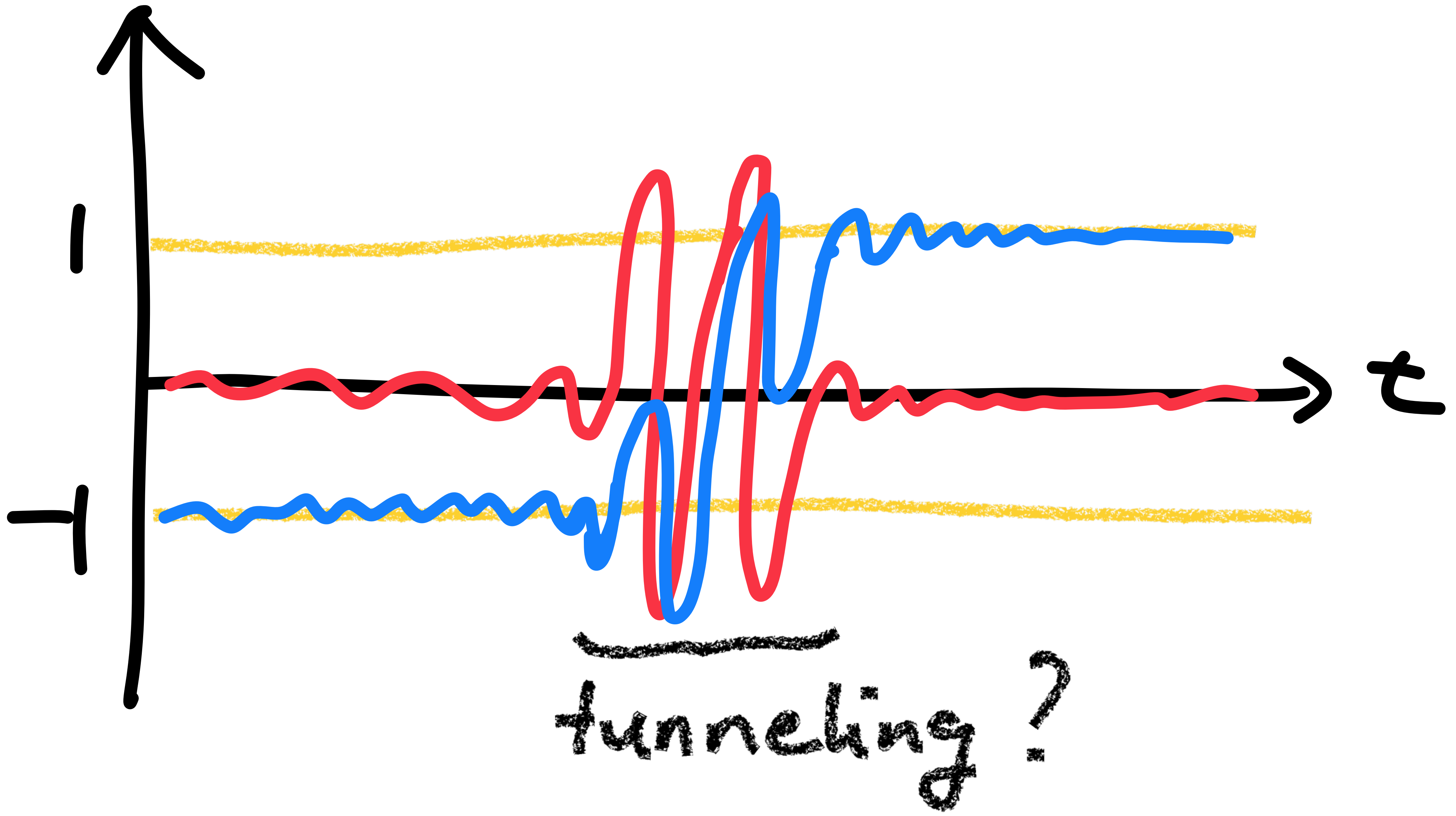


sphaleron ??

To find "tunneling-like" sol., $\frac{n}{T}, \frac{m}{T} \sim \mathcal{O}(1)$.

↳ many complex oscillations

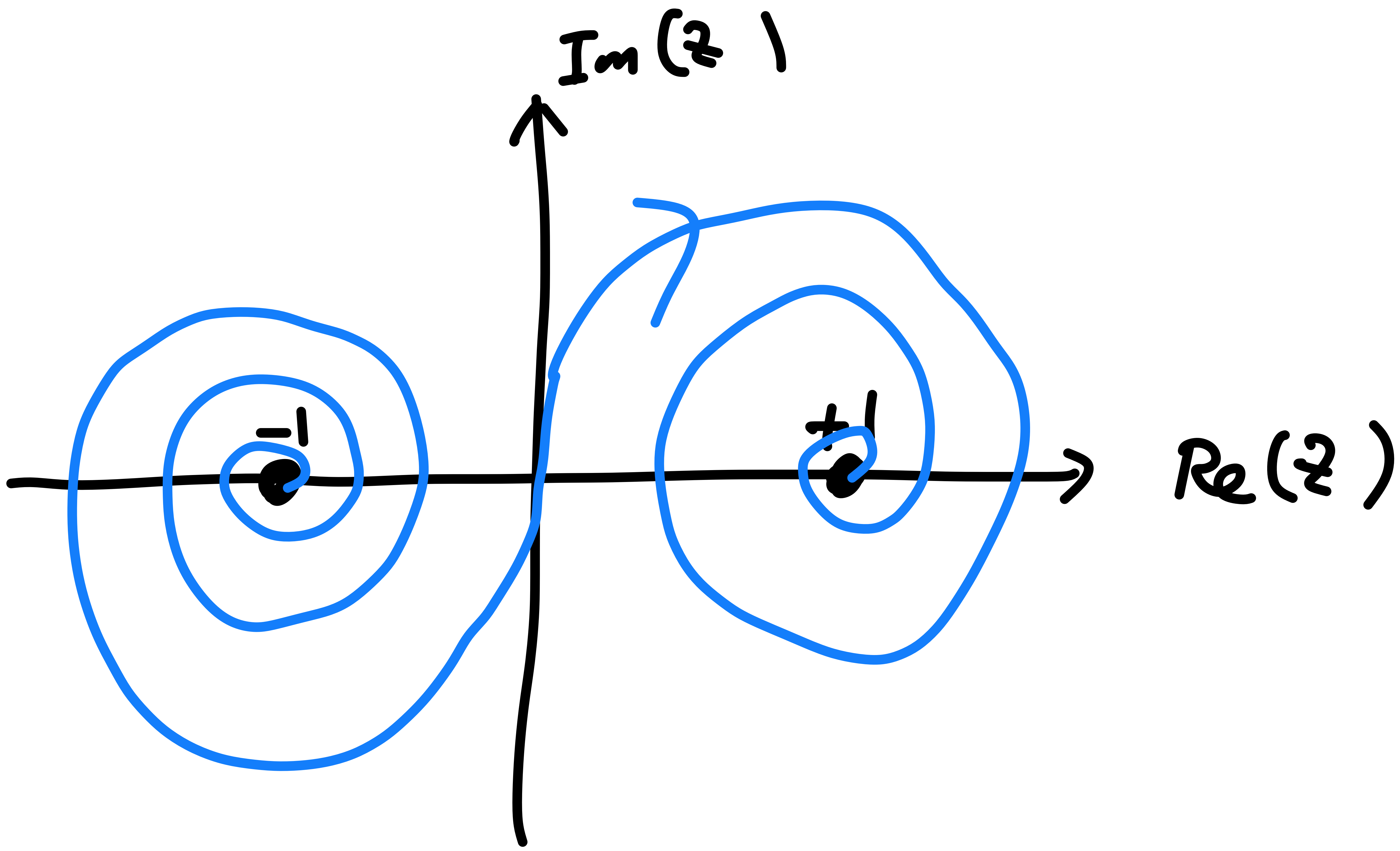
$E \approx 0$.



(cf. Tanizaki, Koike, '14, Cherman, Ünsal, '14)

$I(z) = i S(z) \simeq -\mathcal{O}(1) + i\,(\text{small imaginary part})$.

In a complex plane z, it looks like



This may be a correct semiclassical view of tunneling.

With these solutions,
can we describe tunneling semiclassically?

I honestly don't know!

At least, there are complex classical solutions,
whose amplitude looks reasonable as a tunneling phenomenon

Possible direction

- Double-well looks to be complicated, as tunneling can occur repeatedly.

  ⇒ Can we get better understandings by looking at "single-tunneling" systems ?

- In this study, we used Dirichlet b.c. as initial and final states.

  ⇒ Preparation of better wave functions may enable us to get easier controll of semiclassics.